Advanced Rcpp I

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Local polynomial regression

In this portfolio, we will demonstrate how to perform local polynomial regression both in `R` directly and by using `RcppArmadillo`.

Load the data

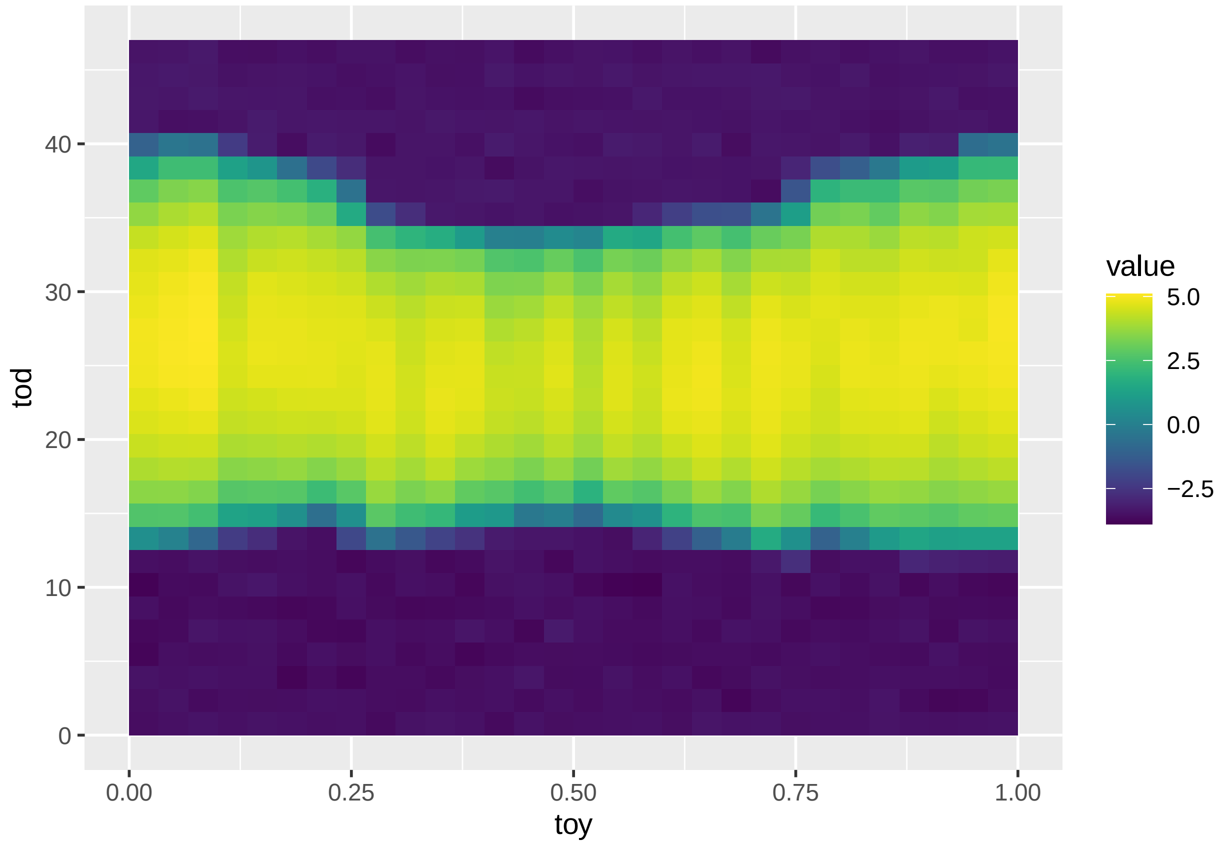
We have the following data set on solar electricity production in Sidney, Australia:

```
library(here)
library(tidyverse)
load(here("portfolios/03_advanced_rcpp_1/data/solarAU.RData"))
head(solarAU)
```

```
##       prod          toy tod
## 8832 0.019 0.000000e+00   0
## 8833 0.032 5.708088e-05   1
## 8834 0.020 1.141618e-04   2
## 8835 0.038 1.712427e-04   3
## 8836 0.036 2.283235e-04   4
## 8837 0.012 2.854044e-04   5
```

We will add a column for the log-transformed production:

```
solarAU$logprod <- log(solarAU$prod+0.01)
# Visualize log-production
library(viridis)
ggplot(solarAU,
       aes(x = toy, y = tod, z = logprod)) +
       stat_summary_2d() +
       scale_fill_gradientn(colours = viridis(50))
```



Q1: Linear regression model

We want to model $\mathbb{E}(y|\mathbf{x})$ where y is the log-production and $\mathbf{x} = \{\text{tod}, \text{toy}\}$. We will use a polynomial regression model of degree 2:

$$\mathbb{E}(y|\mathbf{x}) = \beta_0 + \beta_1 \text{tod} + \beta_2 \text{tod}^2 + \beta_3 \text{toy} + \beta_4 \text{toy}^2 = \tilde{\mathbf{x}}^\top \beta$$

where $\tilde{\mathbf{x}} = \{\text{tod}, \text{tod}^2, \text{toy}, \text{toy}^2\}$.

Using R, we would fit the model as follows:

```r
fit <- lm(logprod ~ tod + I(tod^2) + toy + I(toy^2), data = solarAU)
summary(fit)
```

```
##
## Call:
## lm(formula = logprod ~ tod + I(tod^2) + toy + I(toy^2), data = solarAU)
##
## Residuals:
##     Min      1Q  Median      3Q     Max
## -6.1623 -1.5447  0.6765  1.6280  4.8534
##
## Coefficients:
##               Estimate Std. Error t value Pr(>|t|)
## (Intercept) -6.263e+00  6.422e-02  -97.52   <2e-16 ***
## tod          8.644e-01  4.513e-03  191.53   <2e-16 ***
## I(tod^2)    -1.758e-02  9.286e-05 -189.28   <2e-16 ***
## toy         -5.918e+00  2.207e-01  -26.81   <2e-16 ***
```

```
## I(toy^2)     6.143e+00  2.138e-01   28.74   <2e-16 ***
## ---
## Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
##
## Residual standard error: 2.106 on 17467 degrees of freedom
## Multiple R-squared:  0.6838, Adjusted R-squared:  0.6838
## F-statistic:  9445 on 4 and 17467 DF,  p-value: < 2.2e-16
```

We now want to use `RcppArmadillo` to fit a linear regression model by solving

$$\hat{\beta} = \arg\min_{\beta} \|y - \mathbf{X}\beta\|^2$$

We can define $\mathbf{X}$ and y in R by:

```
X <- with(solarAU, cbind(1, tod, tod^2, toy, toy^2))
y <- solarAU$logprod
```

We can write a function to fit the model using QR decomposition with `RcppArmadillo`:

```
library(Rcpp)
sourceCpp(code = '
// [[Rcpp::depends(RcppArmadillo)]]
#include <RcppArmadillo.h>
using namespace arma;

// [[Rcpp::export(name = "armadillo_lm")]]
vec armadillo_lm(mat& X, vec& y) {
  mat Q;
  mat R;

  qr_econ(Q, R, X);
  vec beta = solve(R, (trans(Q) * y));
  return beta;
}
')
```

We will compare the results and performance with the `lm` function in R:

```
arma_lm_beta <- armadillo_lm(X,y)
max(abs(coef(fit) - arma_lm_beta)) # results are the same
```

```
## [1] 4.360956e-13
```

```
library(microbenchmark)
lm_R <- function() lm(logprod ~ tod + I(tod^2) + toy + I(toy^2), data = solarAU)
lm_arma <- function() armadillo_lm(X,y)
microbenchmark(lm_R(), lm_arma(), times = 500)
```

```
## Unit: microseconds
##       expr      min        lq      mean    median       uq       max neval
##     lm_R() 1483.908 1610.6025 2273.9778 1673.5495 1896.253 45639.025   500
##  lm_arma()  372.457  411.5435  455.1698  436.2725  461.025  4987.983   500
```

The implementation in `RcppArmadillo` is over 6 times faster than the `lm` function in R.

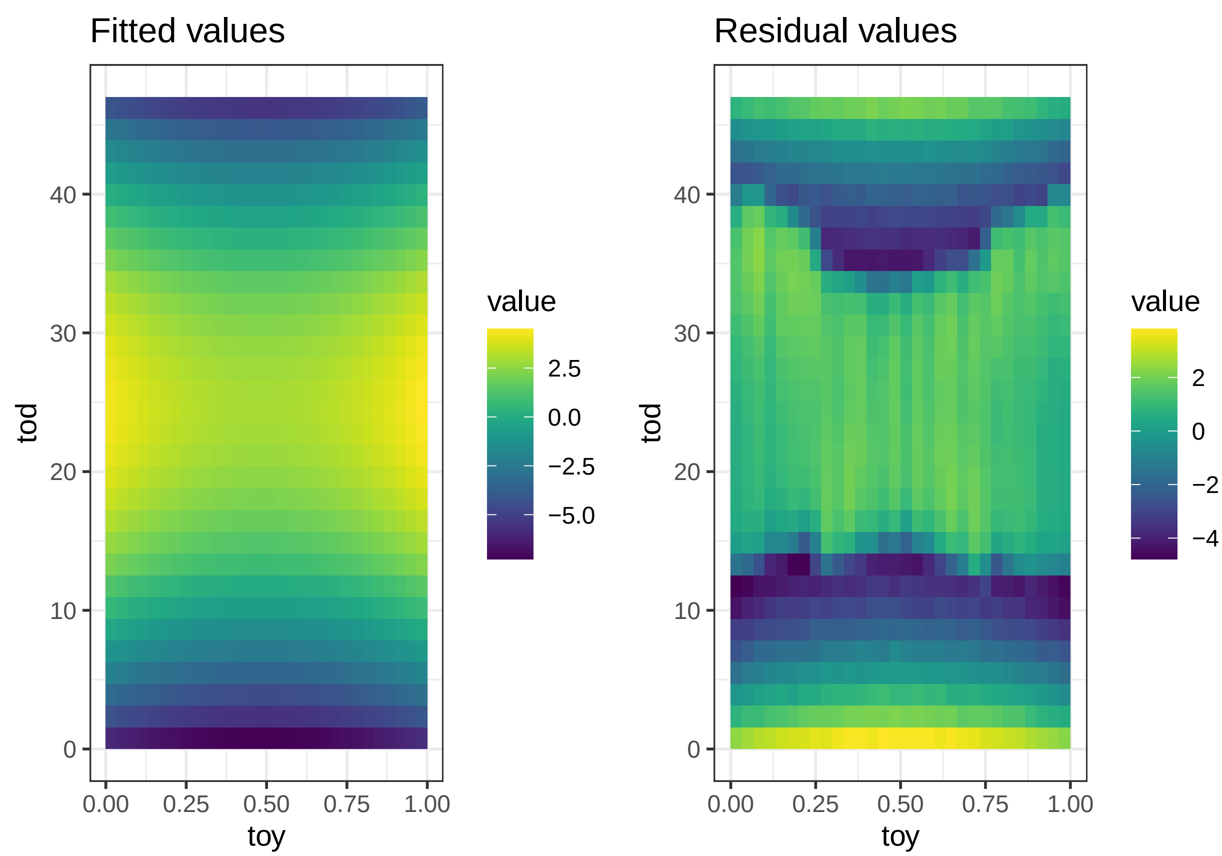
We can now see if the model is a good fit for the data:

```
library(gridExtra)
```

```
solarAU <- solarAU %>%
  mutate(lm_fitted = fit$fitted.values,
         lm_resids = fit$residuals)

fitted_plot <- ggplot(solarAU,
                      aes(x = toy, y = tod, z = lm_fitted)) +
  stat_summary_2d() +
  scale_fill_gradientn(colours = viridis(50)) +
  theme_bw() +
  labs(title = "Fitted values")

resid_plot <- ggplot(solarAU,
                     aes(x = toy, y = tod, z = lm_resids)) +
  stat_summary_2d() +
  scale_fill_gradientn(colours = viridis(50)) +
  theme_bw() +
  labs(title = "Residual values")
grid.arrange(fitted_plot, resid_plot, ncol = 2)
```



The plot of residuals shows a non-linear pattern, suggesting that the model is not a good fit for the data.

Q2: Local least squares regression

We want to try to address this non-linear pattern in the residuals. One possible solution is to use local regression, which fits separate regression models to different subsets of the data. We will now let the regression coefficients be a function of the covariates $\mathbf{x}$, i.e. $\hat{\beta} = \hat{\beta}(\mathbf{x})$. For a given $\mathbf{x}_0$,

$$\hat{\beta}(\mathbf{x}_0) = \arg\min_{\beta} \sum_{i=1}^{n} \kappa_{\mathbf{H}}(\mathbf{x}_0 - \mathbf{x}_i)(y_i - \tilde{\mathbf{x}}_i^\top \beta)^2$$

where κ_H is a density kernel with positive definite bandwidth matrix $\mathbf{H}$.

We can implement a function in R to do this using the Gaussian kernel:

```
library(mvtnorm)
lmLocal <- function(y, x0, X0, x, X, H){
  w <- dmvnorm(x, x0, H)
  fit <- lm(y ~ -1 + X, weights = w)
  return( t(X0) %*% coef(fit) )
}
```

The `lmLocal` function takes the following inputs:

- `y`: response variable
- `x0`: location of the prediction
- `X0` : design matrix at the prediction location
- `x` : locations of the data points
- `X` : design matrix at the data points
- `H` : bandwidth matrix

It returns the fitted values at the prediction location.

We can test this model using a subset of 2000 data points (since fitting it on all 17472 data points would be computationally costly):

```
set.seed(123)
n <- nrow(X)
nsub <- 2e3
# Get 2000 random indices
sub <- sample(1:n, nsub, replace = FALSE)

y <- solarAU$logprod
solarAU_sub <- solarAU[sub, ]
x <- as.matrix(solarAU[c("tod", "toy")])
x0 <- x[sub, ]
X0 <- X[sub, ]
# Using the following H
H <- diag(c(1, 0.1)^2)

# Obtain estimates at each subsampled location
# And check how long that takes
tictoc::tic()
predLocal <- sapply(1:nsub, function(ii){
  lmLocal(y = y, x0 = x0[ii, ], X0 = X0[ii, ], x = x, X = X, H = H)
})
tictoc::toc()
```

```
## 12.247 sec elapsed
```

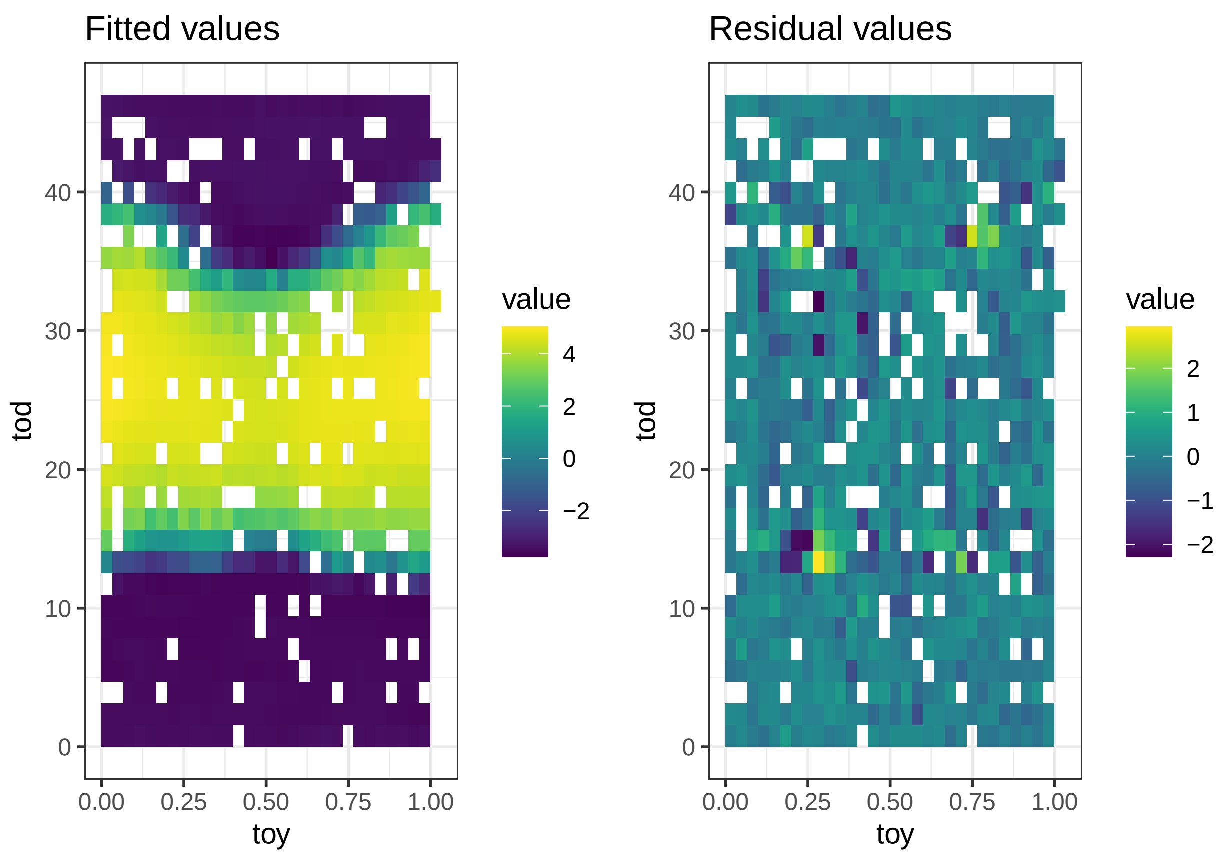
We can see this is a fairly slow process. Let's see how the fit / residuals look:

```
solarAU_sub <- solarAU_sub %>%
  mutate(lmLocal_fitted = predLocal,
         lmLocal_resids = logprod - predLocal)
```

```r
fitted_plot <- ggplot(solarAU_sub,
                      aes(x = toy, y = tod, z = lmLocal_fitted)) +
  stat_summary_2d() +
  scale_fill_gradientn(colours = viridis(50)) +
  theme_bw() +
  labs(title = "Fitted values")

resid_plot <- ggplot(solarAU_sub,
                     aes(x = toy, y = tod, z = lmLocal_resids)) +
  stat_summary_2d() +
  scale_fill_gradientn(colours = viridis(50)) +
  theme_bw() +
  labs(title = "Residual values")

grid.arrange(fitted_plot, resid_plot, ncol = 2)
```



We no longer have a pattern in the residuals, and our fitted values closely resemble our original data.

Let's see if we can implement the local least squares in `RcppArmadillo` to get these good results without the high computational cost. See here for the `armadillo_lm_local.cpp` code file, which depends on two functions included in a header file `armadillo_lm_funcs.h`.

```r
sourceCpp(file = 'armadillo_lm_local.cpp')

arma_predLocal <- armadillo_lm_local(y, x0, X0, x, X, H)
max(abs(predLocal - arma_predLocal)) # results are the same
```

```
## [1] 4.085621e-13
```

```r
predLocal_R <- function() sapply(1:nsub, function(ii){
  lmLocal(y = y, x0 = x0[ii, ], X0 = X0[ii, ], x = x, X = X, H = H)
})
predLocal_arma <- function() armadillo_lm_local(y, x0, X0, x, X, H)
microbenchmark(predLocal_R(), predLocal_arma(), times = 5) # only 5 runs because R is super slow
```

```
## Unit: seconds
##              expr       min       lq      mean    median        uq       max
##     predLocal_R() 10.800570 11.10427 11.321263 11.295741 11.358971 12.046758
##  predLocal_arma()  1.509981  1.51386  1.541455  1.516173  1.578238  1.589021
##  neval
##      5
##      5
```

The RcppArmadillo implementation is almost 7 times faster than the R implementation.

Q3: Choosing bandwidth with cross-validation

We will now use cross-validation to choose the bandwidth matrix **H**. See here for the armadillo_cv_H.cpp code file. We will perform 5-fold cross-validation.

```r
sourceCpp(file = 'armadillo_cv_H.cpp')

# Set of H options for cross-validation
H_options <- list(diag(c(1, 0.1)^2),
                  diag(c(1, 0.01)^2),
                  diag(c(0.9, 0.1)^2))

tictoc::tic()
arma_predLocal_cv <- armadillo_cv_H(y, x0, X0, x, X, H_options, 5)
tictoc::toc()
```

```
## 2.412 sec elapsed
```

We can check which bandwidth matrix **H** was chosen:

```r
arma_predLocal_cv$H
```

```
##      [,1]  [,2]
## [1,]    1 0e+00
## [2,]    0 1e-04
```

We can now see the fits and residuals from using cross-validation to choose the bandwidth matrix:

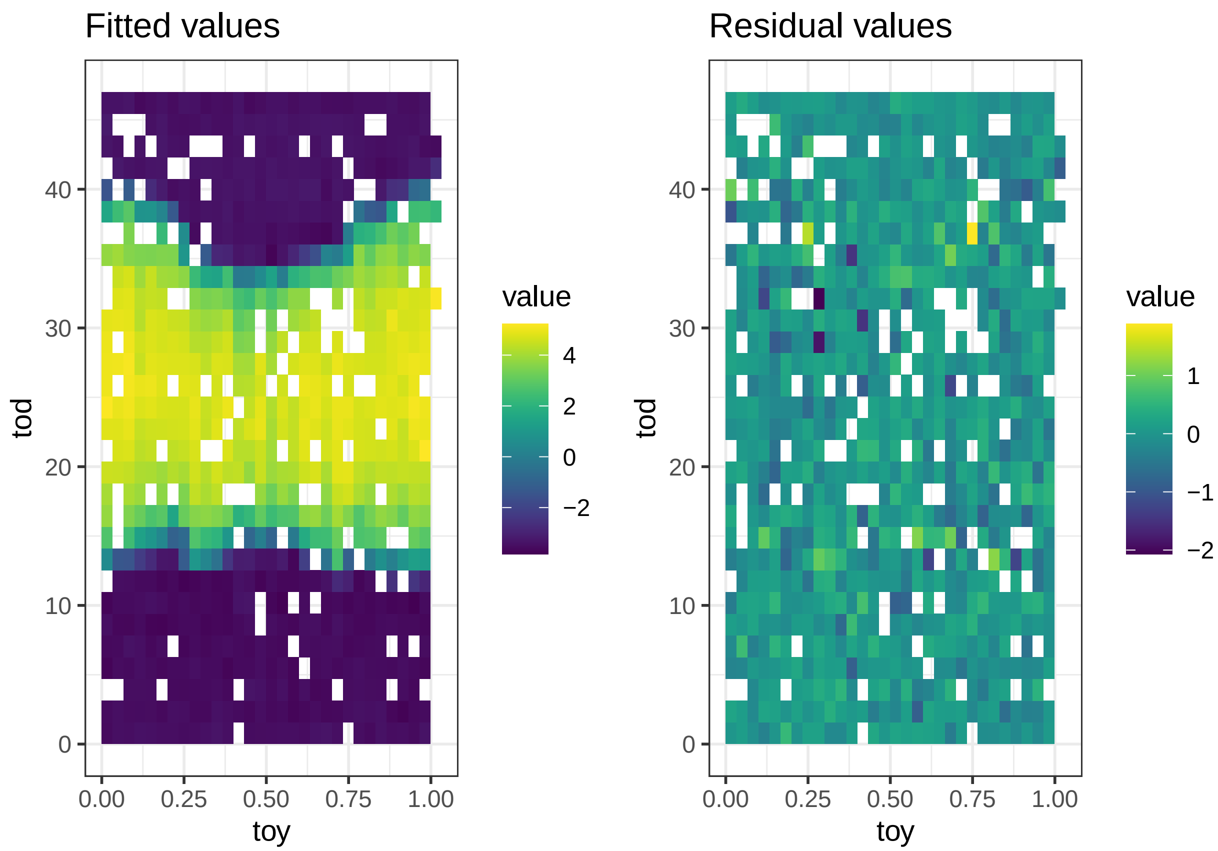
```r
solarAU_sub <- solarAU_sub %>%
  mutate(lmLocal_cv_fitted = arma_predLocal_cv$fitted[,1],
         lmLocal_cv_resids = logprod -  arma_predLocal_cv$fitted[,1])

fitted_plot_cv <- ggplot(solarAU_sub,
                         aes(x = toy, y = tod, z = lmLocal_cv_fitted)) +
  stat_summary_2d() +
  scale_fill_gradientn(colours = viridis(50)) +
  theme_bw() +
  labs(title = "Fitted values")

resid_plot_cv <- ggplot(solarAU_sub,
```

```r
                          aes(x = toy, y = tod, z = lmLocal_cv_resids)) +
  stat_summary_2d() +
  scale_fill_gradientn(colours = viridis(50)) +
  theme_bw() +
  labs(title = "Residual values")

grid.arrange(fitted_plot_cv, resid_plot_cv, ncol = 2)
```



It's hard to visually see the difference between the fits and residuals from the cross-validated bandwidth matrix and the original bandwidth matrix. We can compare the residuals from the two methods:

```r
# MSE from original bandwidth matrix
mse_orig <- mean(solarAU_sub$lmLocal_resids^2)
mse_orig
```

```
## [1] 0.3801064
```

```r
# MSE from cross-validated bandwidth matrix
mse_cv <- mean(solarAU_sub$lmLocal_cv_resids^2)
mse_cv
```

```
## [1] 0.2243705
```

We can see that the mean squared error is lower when using the cross-validated bandwidth matrix.